

Monday 27th June

Time	Session	Location
09:00-19:00	Registration	
10:30-12:00	Workshops	
12:00-13:30	Lunch	
12:15-13:15	Commercial Presentations	
13:30-15:00	Workshops	
16:30-17:00	Opening Ceremony	The Auditorium
17:00-18:00	Plenary Speaker: Jeremy Nicholson Metabolic Profiling in Systems Medicine	The Auditorium
18:00-19:00	Welcome Reception	

Tuesday 28th June

Time	Session	Location
08:50-09:50	Plenary Speaker: Luke O'Neill The intersection between inflammation and metabolism	The Auditorium
09:50-10:30	Tea/Coffee/Posters	
10:30-12:00	Parallel Session 1: Model Organisms <i>Chairs: Choong Hwan Lee and Carl Ng</i>	The Auditorium
10:30-10:55	2459 When NMR spectroscopy is not such a DOSY alternative – using NMR to model complex formation and the origins of metabolism Julian Griffin, University of Cambridge, UK	
10:55-11:10	2304 Mapping metabolism in the parasite Trypanosoma brucei using U-13C-labelled amino acids and LC-MS Fiona Achcar, University of Glasgow, UK	
11:10-11:25	2551 The Time is Right to Focus on a Model Organism Database, Christoph Steinbeck, European Bioinformatics Institute, UK	
11:25-11:40	2071* The role played by CYP6G1 in the metabolism of imidacloprid and its 5-hydroxy and olefin metabolites in Drosophila melanogaster Roberto Fusetto, The University of Melbourne, Australia	
11:40-11:55	2237* Spatio-temporal metabolomics of tumor organoids treated with chloroquine Andrew Palmer, EMBL, Germany	
10:30-12:00	Parallel Session 2: Biomarkers in Nutrition Research <i>Chairs: Kati Hanhineva and Henrik Antti</i>	The Liffey A
10:30-10:55	2298 A Metabolome Wide Association Study of fruit intakes Linda Oude Griep, Imperial College London, UK	
10:55-11:10	2365 Large-scale metabolomics to assess pharmacokinetics of conjugated black tea catabolites in human plasma	

	Ric de Vos, Plant Research International, Wageningen-UR, Netherlands	
11:10-11:25	2597* New classification and validation system for intake biomarkers to improve assessment of food intake and nutritional status – A FoodBALL project goal Giulia Pratico, University of Copenhagen, Denmark	
11:25-11:40	2134 An integrated approach for the identification of predictive markers of type 2 diabetes Blandine Comte, INRA, Clermont-Ferrand, France	
10:30-12:00	Parallel Session 3: CVD/Diabetes <i>Chair: David Wishart and Oscar Yanas</i>	The Liffey B
10:30-10:55	2111 Metabolomic Profiling of Patients with Congenital Adrenal Hyperplasia Reveals Novel Biomarkers for Glucocorticoid Action David Watson, University of Strathclyde, Scotland	
10:55-11:10	2338 Metabolomics and proteomics analysis of vitreous humor from healthy, non-proliferative and proliferative diabetic retinopathy patients Miriam Navarro, University of Rovira and Virgili, Spain	
11:10-11:25	2358* Identification of serum metabolites associated with risk of type 2 diabetes by untargeted metabolomics approach: A nested case control study Lili Xiu, Academia Sinica, Taiwan	
11:25-11:40	2532 Metabolite profiling of plasma and tissues from mouse models of diabetes at different stages of disease development Pieter Giesbertz, Technical University of Munich, Germany	
11:40-11:55	2090* Metabolomics reveals the importance of the pre-conception metabolic state for pregnancy metabolism and programming offspring health Christian Hellmuth, Ludwig Maximilian University of Munich, Germany	
12:00-13:30	Lunch/Posters	
Commercial Symposia	Commercial Presentations	
13:30-15:00	Parallel Session 4: Network and Pathway Analysis for Metabolomics <i>Chairs: Fabien Jourdan and Egon Willighagen</i>	The Auditorium
13:30-14:00	Keynote Speaker Building the Killer App for Modeling Metabolism: from ModelSEED to KBase Matt DeJongh, Hope College, Michigan, USA	
14:00-14.15	2345	

	Isotope tracer-based metabolomics applied to non-steady state circadian systems Seth Rhoades, University of Pennsylvania, USA	
14:15-14:30	2403 Carbon Flux Signatures of Mycobacterium tuberculosis Katharina Nöh, IBG-1: Biotechnology, Forschungszentrum Jülich, Germany	
14:30-14:45	2153 TTFD: a metabolic network-based guidance tool for the setup and interpretation of stable isotope metabolomics experiments Dries Verdegem, VIB-KU Leuven, Belgium	
14:45-15:00	2346* Evidence for a chemically enabled non-enzymatic origin of the Krebs cycle Markus Keller, Division of Biological Chemistry, University of Innsbruck, Austria	
13:30-15:00	Parallel Session 5: Metabolic Phenotyping in Health and Disease <i>Chairs: Matej Oresic and Nichole Reisdorph</i>	The Liffey A
13:30-14:00	Keynote Speaker Personalized Medicine in Human Space Flight: What Elite Athletes can Teach us About Molecular Deficits that affect Astronaut Health and Performance Michael Schmidt, Colorado State University, US	
14:00-14.15	2563 Metformin metabolomic profiles to inform pharmacogenomic discovery Matthew Breitenstein, Mayo Clinic, USA	
14:15-14:30	2591 Pharmacometabolomics: Enabling Tool for Precision Medicine Rima Kaddurah-Daouk, Duke University Medical Center, USA	
14:30-14:45	2311 Lipid mediator profiling for identifying sub-phenotypes of respiratory disease Craig Wheelock, Karolinska Institute, Sweden	
14:45-15:00	2328 Metabolomics profiling identifies gender-enhanced upregulation of oxidative stress in COPD Shama Naz, Karolinska Institute, Sweden	
13:30-15:00	Parallel Session 6: Crop quality improvement and food sustainability <i>Chairs: Robert Hall and Doris Jacob</i>	The Liffey B
13:30-14:00	Keynote Speaker Variability in fruit metabolites in tomato: leads for understanding the underlying biology and to improve fruit quality Tony Granell, Polytechnic University, Valencia, Spain	
14:00-14.15	2388 Application of LC - Data independent acquisition (DIA) - digital archiving (DA) mass spectrometry for mycotoxin and	

14:15-14:30	metabolite profiling of silage Mark Sumarah, Agriculture and Agri-Food Canada 2300 Multi-platform metabolomics analyses of a broad collection of fragrant and non-fragrant rice varieties reveals the high complexity of grain quality characteristics Roland Mumm, Wageningen University and Research, Business Unit, Netherlands	
14:30-14:45	2054 Fruit position within pear trees impacts ripening and associated metabolism after harvest David Rudell, USDA-ARS, USA	
14:45-15:00	2173 Metabolomics to assess the potential of fermented fruit/vegetable by-products as a new source of functional foods Ninna Granucci, The University of Auckland, New Zealand	
15:00-15:30	Tea/Coffee/Posters	
15:30-17:00	Parallel Session 7: Nutrition and Metabolism <i>Chairs: Ines Thiel and Jules Griffin</i>	The Auditorium
15:30-16:00	Keynote Speaker Process Metabolomics: living systems under “direct” observation. Soren Engelsen, University of Copenhagen, Denmark	
16:00-16:15	2506 Evolution of Gut Microbiota:Host co-metabolic processes determined both by term and mode of birth in the INFANTMET Cohort Cian J. Hill, University College Cork, Ireland	
16:15-16:30	2088 The effect of plant sterols and different low doses of omega-3 fatty acids from fish oil on lipoprotein subclasses Doris Jacobs, Unilever R&D, The Netherlands	
16:30-16:45	2398 The application of lipid profiling to understand dietary fat metabolism in breast-fed infants Albert Koulman, MRC Human Nutrition Research, UK	
15:30-17:00	Parallel Session 8: Environmental Metabolomics <i>Chairs: Carl Ng and Annick Moing</i>	The Liffey A
15:30-16:00	2246 MetFish: A suite of chemoselective tags combined with tandem mass spectrometry for quantitative and comprehensive metabolomics analyses in extreme environments Thomas Metz, Pacific Northwest National Laboratory, USA	
16:00-16:15	2044* High resolution mass spectrometry for understanding biochemical impacts in fish exposed to complex mixtures of environmental contaminants Jonathan Mosley, US Environmental Protection Agency, USA	
16:15-16:30	2069*	

	Mass spectrometry-based lipidomics to study effects of naphthalene on various organs of mice Ping-Chun Hsieh, National Taiwan University, Taiwan	
16:30-16:45	2203 Towards a fully-automated extraction of polar and apolar metabolites from low mass tissue samples Jelena Sostare, University of Birmingham, UK	
16:45-17:00	2030 Responses in the metabolome & lipidome of marine copepods induced by climate-related food deprivation Ulf Sommer, University of Birmingham, UK	
15:30-17:00	Parallel Session 9: Advances in Statistical Tools <i>Chairs: Age Smilde and David Broadhurst</i>	The Liffey B
15:30-15:55	2330 A Novel Method for Power Analysis and Sample Size Determination in Metabolic Phenotyping Tim Ebbels, Imperial College London, UK	
15:55- 16:10	2193 Exploring metabolomic data from designed experiments using ANOVA-Multiblock Orthogonal Partial Least Squares Julien Boccard, University of Geneva, Switzerland	
16:10-16:25	2035 Batch correction in the presence of non-detects Ron Wehrens, Wageningen UR, Netherlands	
16:25-16:40	2194 Dealing with sample dependency in metabolomics studies Pär Jonsson, Umeå University, Sweden	
16:40-16:55	2286 Batch correction strategies to reduce non-biological variation in large-scale metabolic profiling Fumiaki Imamura, University of Cambridge, UK	
17:15-18:45	Poster Session 1	
19:00-20:30	EMN Reception	

Wednesday 29th June

Time	Session	Location
08:50-09:50	Plenary Speaker: Ines Thiel Modelling of Human Metabolism	The Auditorium
09:50-10:30	Tea/Coffee/Posters	
10:30-11:50	Parallel Session 10: Early Career Session 1 <i>Chairs: Aoife O’Gorman and Fidele Tugizimana</i>	The Auditorium
10:30-10:45	2154 Metabolic profiling of total physical activity and sedentary behavior in community-dwelling men Kota Fukai, Keio University, Japan	
10:45-11:00	2284 Metabolomic profiles in different models of hepatocytes	

	proliferation: partial hepatectomy and mitogen-induced hyperplasia Laura Tronci, University of Cagliari, Italy	
11:00-11:15	2548 NMR spectroscopy detects metabolite differences between culture media of hepatitis C virus negative and positive cells after harvest Gaëlle Diserens, DCR & DIPR, University of Bern, Switzerland	
11:15-11:30	2524 Stable isotope assisted evaluation of different extraction solvents for metabolomics of cereals using LC-HRMS Maria Doppler, University of Natural Resources and Life Sciences, Vienna, Austria	
11:30-11:45	2366 High quality metabolomics Mass Spectrometry Imaging using sputtered gold nanolayers Sonia Torres, Institut Investigacio Sanitaria Pere Virgili, Spain	
10:30-11:50	Parallel Session 11: Early Career Session 2 <i>Chairs: Stacey Reinke and Justin van der Hooft</i>	The Liffey B
10:30-10:45	2415* Metabolomic based identification of clusters that reflect dietary patterns Helena Gibbons, University College Dublin, Ireland	
10:45-11:00	2040* Determination of the differences in metabolite profile in Sclerocarya birrea from different geographical origin and the effect on in-vitro glucose uptake activity Cynthia Marokane, University of South Africa	
11:00-11:15	2424 In the quest of robust biomarkers for inflammatory bowel disease phenotypes using GC×GC-HRTOFMS Nicolas Di Giovanni, University of Liège, Belgium	
11:15-11:30	2229* Crosstalk between astrocytes and motor neurons: a metabolomics study Blandine Madji Hounoum, Université François-Rabelais, France	
11:30-11:45	2368* Novel indicators of severe acute malnutrition in a cohort of Nigerian children identified through untargeted metabolomics Amy McMillan, University of Western Ontario, Canada	
11:50-13:30	Lunch/Posters Commercial Presentations	
13:30-15:00	Parallel Session 12: New Approaches for Identification of Metabolites Applying NMR and MS <i>Chairs: Michael Witting and Rick Dunn</i>	The Auditorium
13:30-14:00	Keynote Speaker New approaches for NMR-based, hybrid NMR/MS, and	

	nanoparticle-assisted metabolomics Rafael Brüscheiler, The Ohio State University, US	
14:00-14:15	2106 New Approaches to NMR-Based Metabolite Identification Jeremy Everett, University of Greenwich, UK	
14:15-14:30	2447 mzCloud: An online substructural database of spectral trees for the identification of metabolites Robert Mistrik, HighChem, Slovakia	
14:30-14:45	2109 Discovery of regulated metabolite families in untargeted metabolomics studies Gerd Balcke, Leibniz Institute of Plant Biochemistry, Germany	
14:45-15:00	2397 FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry Theodore Alexandrov, EMBL, Germany	
13:30-15:00	Parallel Session 13: Green Systems Biology <i>Chairs: Wolfram Weckwerth and Darren Creek</i>	The Liffey A
13:30-14:00	Keynote Speaker The integration of physiological, proteomic, and metabolomic levels reveals new adaptive and stress-responsive mechanisms in Pinus Luis Valledor, University of Oviedo, Spain	
14:00-14:15	2168 Metabolomics and methanogenic potential - reducing agricultural greenhouse gases Simone Rochfort, AgriBio, La Trobe University, Australia	
14:15-14:30	2383 Novel pathways, metabolites and bioactivity – A fresh look at salicinoid biosynthesis through NMR-MS metabolomics Jane Ward, Rothamsted Research, UK	
14:30-14:45	2441 Metabolomics and inverse modelling of the AMPK-TOR crosstalk in plants and animals Wolfram Weckwerth, University of Vienna, Austria	
14:45-15:00	2192 Metabolic mapping in plants: LAESI-MS imaging Robert Hall, Wageningen UR, Netherlands	
13:30-15:00	Parallel Session 14: Metabolomics Profiling in Cancer <i>Chairs: Lars Dragsted and Krista Zanetti</i>	The Liffey B
13:30-13:45	2119 Serum metabolomic profiling of prostate cancer risk in the Prostate, Lung, Colorectal and Ovarian Cancer Screening (PLCO) Trial Demetrius Albanes, US National Cancer Institute, USA	
13:45-14:00	2287 Brain tumour: Can LC-MS-based metabolomics reveal the tumour invasive margin? Dong-Hyun Kim, University of Nottingham, UK	

14:00-14:15	2594 DESI-Imaging of inflammatory markers for cancer Renata Soares, Imperial College London, UK	
14:15-14:30	2041 Metabolomics study of early hepatocarcinogenesis from mice model: role of methylation and energy metabolism Peiyuan Yin, Dalian Institute of Chemical Physics, China	
14:30-14:45	2500* Myc linked to aberrant lipid metabolism in lung cancer by mass spectrometry imaging Zoe Hall, University of Cambridge, UK	
14:45-15:00	2353 Plasma metabolomics for prognostic biomarker development in pancreatic cancer Amrita Cheema, Georgetown University, USA	
15:00-15:30	Tea/Coffee/Posters	
15:30-17:00	Parallel Session 15: Foodomics and Food Quality <i>Chairs: Karsten Hiller and Cristina Andres Lacueva</i>	The Auditorium
15:30-16:00	Keynote Speaker Combining metabolomics and genomics to dissect rice quality, and provide robust and trait-relevant tools to rice breeders Melissa Fitzgerald, University of Queensland, Australia	
16:00-16:15	2410 Global untargeted metabolomics approach to reveal metabolic shifts during postharvest cold storage of 'Kinnow' Mandarin Manpreet Saini, National Agri-Food Biotechnology Institute, Mohali, India	
16:15-16:30	2138 What makes a peanut, a peanut? Elucidating the metabolome of the raw peanut seed Claire Klevorn, North Carolina State University, USA	
16:30-16:45	2068 Wine and grape juice lipidomics: the impact of juice lipids on wine properties Silas Villas-Boas, University of Auckland, New Zealand	
16:45-17:00	2222 Real time detection of fish fraud using rapid evaporative ionisation mass spectrometry (REIMS) Connor Black, Queens University Belfast, UK	
15:30-17:00	Parallel Session 16: Impact of Metabolomics in Clinical Medicine 1 <i>Chairs: Louise Kenny and Jerzy Adamski</i>	The Liffey A
15:30-16:00	Keynote Speaker Metabolomics and Epidemiology: Building Infrastructure and Leveraging Resources to Accelerate Scientific Discovery Krista Zanetti, National Cancer Institute, US	
16:00-16:15	2565 Direct from Sample Microbial Metabolomics using Rapid Evaporative Ionisation Mass Spectrometry (REIMS)	

16:15-16:30	Simon Cameron, Imperial College London, UK 2285 The metabolic signature of stored red blood cells can be used for assessing the quality of red cell concentrate units during the storage	
16:30-16:45	Giuseppe Paglia, European Academy of Bolzano/Bozen, Italy 2561* Linking the gut microbiome, blood metabolites and Volatile organic compounds in breath	
16:45-17:00	Agnieszka Smolinska, Maastricht University, Netherlands 2503 How humanisation of the liver affects metabolism in the mouse brain	
15:30-17:00	Parallel Session 17: Computational MS <i>Chairs: Steffen Neumann and Sebastian Böcker</i>	The Liffey B
15:30-16:00	Keynote Speaker Generalized methods for targeted 13C metabolic flux analysis	
16:00-16:15	Nicola Zamboni, ETH, Switzerland 2326 IFrID: A Novel In-Source Fragmentation Detection and Deconvolution Algorithm for LC-MS Metabolomics Data	
16:15-16:30	Tytus Mak, National Institute of Standards and Technology, USA 2416 Towards enhanced plant metabolomics by combining 13C-labeling assisted workflows to study the metabolic defense of wheat against Fusarium	
16:30-16:45	Christoph Bueschl, BOKU University Vienna, Austria 2023 Significance of metabolite identifications from searching mass spectral libraries	
16:45-17:00	Franziska Hufsky, Friedrich Schiller University Jena, Germany 2077 Confidence score for metabolite identifications from structural library search	
17:00-18:30	Marcus Ludwig, Friedrich Schiller University Jena, Germany	
17:00-18:30	Poster Session 2	
20:00-23:30	Conference Dinner	

Thursday 30th June

Time	Session	Location
09:00-10:30	Parallel Session 18: Abiotic and Biotic Stresses in Plants	The Auditorium

	<i>Chairs: Ute Roessner and Tsutomu Masujima</i>	
09:00-09:30	Keynote Speaker Metabolite profiles of field grown maize leaves subjected to combined abiotic stresses and its relationship to grain yield performance Toshihiro Obata, Max-Planck-Institute of Molecular Plant Physiology, Germany	
09:30-09:45	2180* Non-targeted and targeted metabolomic approaches reveal differences in legume chemistry before and after infestation with pea aphid host races Carlos Sanchez Arcos, Max Planck Institute, Germany	
09:45-10:00	2082 Comparative metabolite profiling from growth chamber, environmental simulation chamber or field trial experiments investigating cold acclimation of 49 natural accessions of Arabidopsis thaliana Ellen Zuther, Max Planck Institute, Germany	
10:00-10:15	2142 Metabolite profiling of shoot extracts, root extracts, and root exudates of rice under nitrogen and phosphorus deficiency Keitaro Tawaraya, Yamagata University, Japan	
10:15-10:30	2002 A metabolomics approach to study the "war" between plants and insects - Identification of plant gene functions and their consequences in herbivory insects Aiko Barsch, Bruker Daltonics, Germany	
09:00-10:30	Parallel Session 19: New Development in Instruments and Techniques	The Liffey A
	<i>Chairs: Dan Bearden and Tim Ebbels</i>	
09:00-09:30	Keynote Speaker Mass spectrometric strategy for clinical metabolomics Tuulia Hyötyläinen, Steno Diabetes Centre, Denmark	
09:30-09:45	2226 Stable isotope-labeled yeast extracts as internal standard for LC-MS/MS based amino acid quantification in samples of human origin Gerrit Hermann, ISOTopic solutions, Austria	
09:45-10:00	2324 Addition of drift-tube ion mobility to liquid chromatography-mass spectrometry workflows: examining the potential for cellular metabolomics Tim Causon, University of Natural Resources and Life Sciences, Austria	
10:00-10:15	2238 Optimus + `ili: software for LC-MS based untargeted spatial metabolomics in 2D and 3D Ivan Protsyuk, EMBL, Germany	
10:15-10:30	2466 Spatial Metabolomics: MALDI Mass Spectrometry Imaging	

of Plant Metabolites

Berin Boughton, University of Melbourne, Australia

09:00-10:30	Parallel Session 20: Impact of Metabolomics in Clinical Medicine 2 <i>Chairs: Blandine Comte and Lorraine Brennan</i>	The Liffey B
09:00-09:30	Keynote Speaker Metabolic rewiring of macrophages during inflammation: How metabolism provides antimicrobial activity and regulates inflammation Karsten Hiller, Luxembourg Centre for Systems Biomedicine	
09:30-09:45	2436 Origin of plasma acylcarnitines in humans during fasting and exercise Miriam Hoene, University Hospital Tuebingen, Germany	
09:45-10:00	2390 Medium-throughput metabolomics screening identifies modes of action for novel antimalarials Darren Creek, Monash Institute of Pharmaceutical Sciences, Australia	
10:00-10:15	2343* Brain metabolomics identifies involvement of unsaturated fatty acid metabolism in “asymptomatic Alzheimer’s disease” Stuart Snowden, Kings College London, UK	
10:15-10:30	2453 Serine, threonine metabolic pathways associated with HDL-C response to niacin treatment Sony Tuteja, University of Pennsylvania Perelman School of Medicine, USA	
10:30-10:50	Tea/Coffee	
10:50-11:50	Parallel Session 21: Metabolomics in Early Life <i>Chairs: Hwang Geum-Sook and Aifric O Sullivan</i>	The Auditorium
10:50-11:05	2045* Integration of metabolomic and genome-wide transcriptomic networks in pregnant women reveals biological pathways associated with pre-eclampsia Rachel Kelly, Brigham and Women's Hospital Harvard Medical School, USA	
11:05-11:20	2384 Early serum biomarkers to predict risk of third trimester placental abruption Susan Sumner, RTI International, USA	
11:20-11:35	2396* The placental mitochondrial metabolome suggests the importance of lipid metabolism in pre-eclampsia Ting-Li Han, University of Auckland, New Zealand	
11:35-11:50	2313* Childhood obesity and insulin resistance, metabolomics strategies unveil early onset metabolic alteration and the influence of sex Annalaura Mastrangelo, Universidad San Pablo CEU, Spain	

10:50-11:50	Parallel Session 22: Metabolomic Analysis of Challenge Tests <i>Chair: Hannelore Daniel</i>	The Liffey A
10:50-11:05	2583 Visualizing and exploring the dynamics of the human metabolome: the Humet 2.0 data repository Gabi Kastenmüller, Helmholtz Zentrum München, Germany	
11:05-11:20	2589 Dynamic Response of the Human Metabolome to Environmental Stimuli through Comprehensive Metabolomic Profiling – the Humet 2.0 Study Robert Mohny, Metabolon, Inc., USA	
11:20-11:35	2402 Stability of human plasma “metabotypes” in response to dietary challenges Jarlei Fiamoncini, Technical University of Munich, Germany	
11:35-11:50	2477 The dynamic range of the human metabolome revealed by challenges: a non-target view Karsten Suhre, Weill Cornell Medicine , Qatar	
10:50-11:50	Parallel Session 23: Metabolomics for Disease Biomarkers <i>Chair: Michael Schmidt</i>	The Liffey B
10:50-11:05	2163 Metabolic phenotyping to predict mortality and individualise treatment and transplant candidacy in patients with cirrhosis Muireann Coen, Imperial College London, UK	
11:05-11:20	2128 Human serum metabolites associate with severity and patient outcomes in traumatic brain injury Matej Oresic, Turku Centre for Biotechnology, Finland	
11:20-11:35	2375 GC-MS metabolomics towards a putative urinary biosignature for Tuberculous Meningitis in children Shayne Mason, North-West University, SA	
11:35-11:50	2046 Integrating metabolomics and transcriptomics in the study of asthma severity Jessica Lasky-Su, Brigham and Women's Hospital Harvard Medical School, USA	
12:00-12:40	Plenary Speaker: Tsutomu Masujima Direct metabolomics for plant single cells	The Auditorium
12:40-13:30	Closing Ceremony	The Auditorium

*indicates Early Career Travel Award Winners